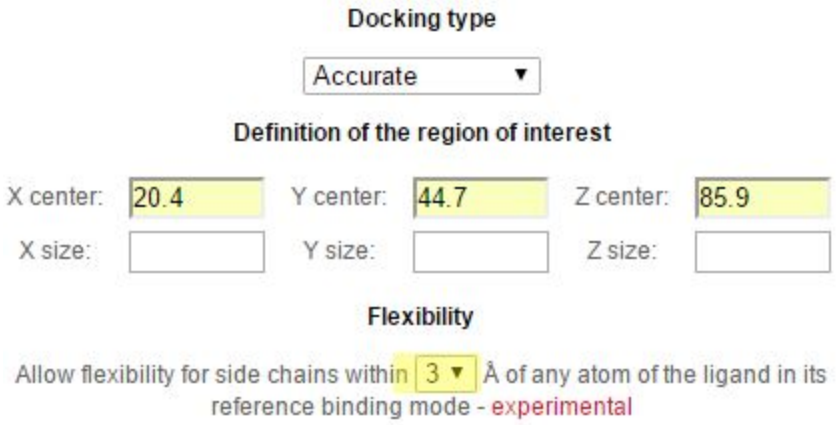
# Step 3.3 - Place the ligand into the protein

1. Go to http://www.swissdock.ch/docking
2. In the target selection, upload the file "<PDB>_relaxed.pdb"
3. In the ligand selection, need to upload the "LIG.pdb" file created in the prev step. **BUT** - need to upload it in MOL2 format. How to save LIG.pdb as LIG.mol2:
    a. Open chimera
    b. Open LIG.pdb file
    c. Click file -> save MOL2

    Then upload the LIG.mol2 file to the site.
4. Enter description and email address
5. Click on "show extra parameters" and edit the options. Should look like:




6. Wait for mail with the results….
7. Open mail and go to results page. Download the results with clicking the icon

Download your predictions file

8. Get a zip file. Unzip it and then untar it. (just run the commands:)

```
unzip <zip file name>
tar xf complexes.tar.xz
```

9. Get your desired result (usually will be complex0_0) and open it in chimera. In chimera do:
    a. Select ->structure -> ligand
    b. Select -> Invert (selected models)
    c. Action -> Atoms/bonds -> delete
    d. Save as "LIG_positioned.pdb"
10. Open "LIG_positioned.pdb" in text editor and make sure it look something like that:
    **Note:** in every row it should be LIG X and not LIG A or any other thing… and try to not

add extra spaces because it shitted the pdb file.

```
HETATM    4  O1  LIG X   1      20.275  42.930  84.368  1.00  0.00           O
HETATM    5  C3  LIG X   1      20.374  45.621  83.764  1.00  0.00           C
HETATM    6  C4  LIG X   1      20.502  45.266  82.280  1.00  0.00           C
HETATM    7  O2  LIG X   1      19.757  45.934  81.513  1.00  0.00           O
HETATM    8  O3  LIG X   1      21.390  44.421  81.988  1.00  0.00           O
HETATM    9  O4  LIG X   1      22.193  42.940  85.588  1.00  0.00           O
HETATM   10  H1  LIG X   1      23.030  45.107  83.384  1.00  0.00           H
```